

2-Propanol-2-d1
3972-26-7 | DTXSID70480714

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 90.0 °C

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Isopropanol</div> <div>Measured: 82.3</div> <div>Predicted: 90.0</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 97.2</div> <div>Predicted: 96.5</div>	<div>Image not found</div> <div>Ethyl hydroperoxide</div> <div>Measured: 95.0</div> <div>Predicted: 99.9</div>
<div>Image not found</div> <div>tert-Butyl alcohol</div> <div>Measured: 82.4</div> <div>Predicted: 97.0</div>	<div>Image not found</div> <div>2-Chloroethanol</div> <div>Measured: 129</div> <div>Predicted: 122</div>	